

Abstract Submitted
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Cyanide Nanotubes YINA MO, EFTHIMIOS KAXIRAS, Harvard University — The discovery of carbon nanotubes (CNTs) has given birth to an entire field devoted to the study of these one-dimensional (1D) nano-scale structures with extraordinary properties and tremendous promise for applications. To mention but a few, single wall carbon nanotubes are reported to exhibit Luttinger liquid behavior and proximity-induced superconductivity, and can be efficient hydrogen storage systems. The electronic properties of a carbon nanotube are fully determined by its helicity and range from metallic to semiconducting. However, when growing nanotubes, it is not possible to control the helicity; thus, carbon nanotube properties are not a result of design but luck. To overcome this limitation, Cohen and coworkers predicted the existence of insulating boron-nitride nanotubes (BNTs) and Zettl produced such tubes experimentally; these tubes are semiconducting and their properties vary less with helicity. Here we propose another type of structurally simple and energetically stable nanotubes consisting of transition metals and cyanide units, which are semiconductors with large band gaps ($\sim 2 - 3$ eV). Using first-principles calculations, we study the properties of these nanotubes and find that their helicity does not significantly affect the electronic band gap. The nature of bonding in these systems singles out a particular helicity as energetically more stable, suggesting that only one type of tube will be predominantly formed with well defined electronic properties.

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